

# Optimization for Quantum Systems

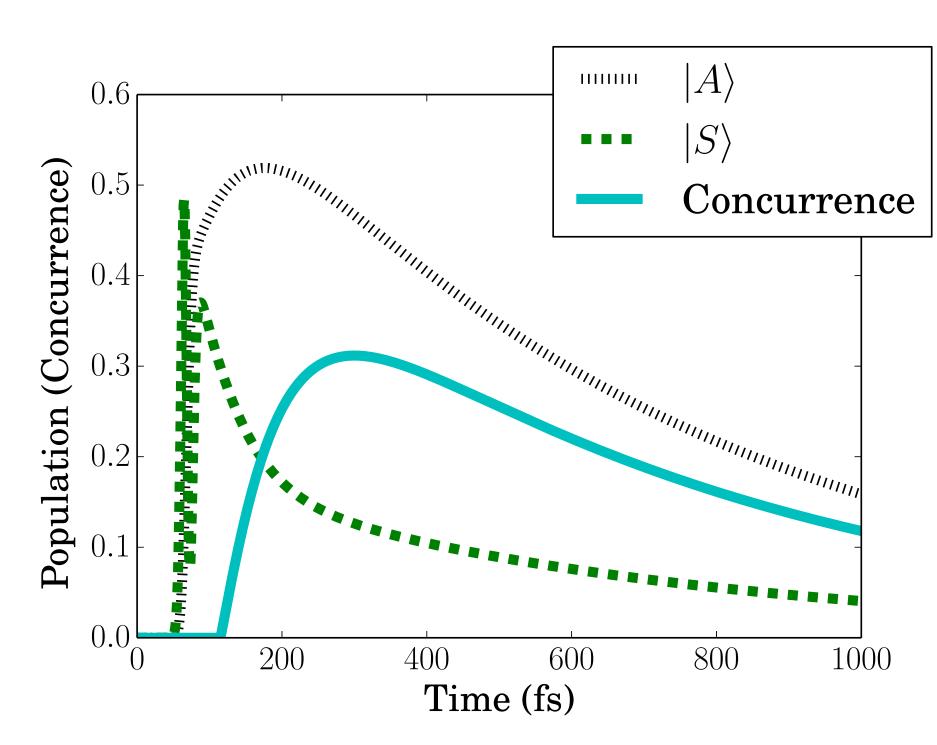
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Maximizing concurrence

- Concurrence is a measure of entanglement of a quantum system
- Concurrence of two quantum dots excited by a single optical laser pulse:



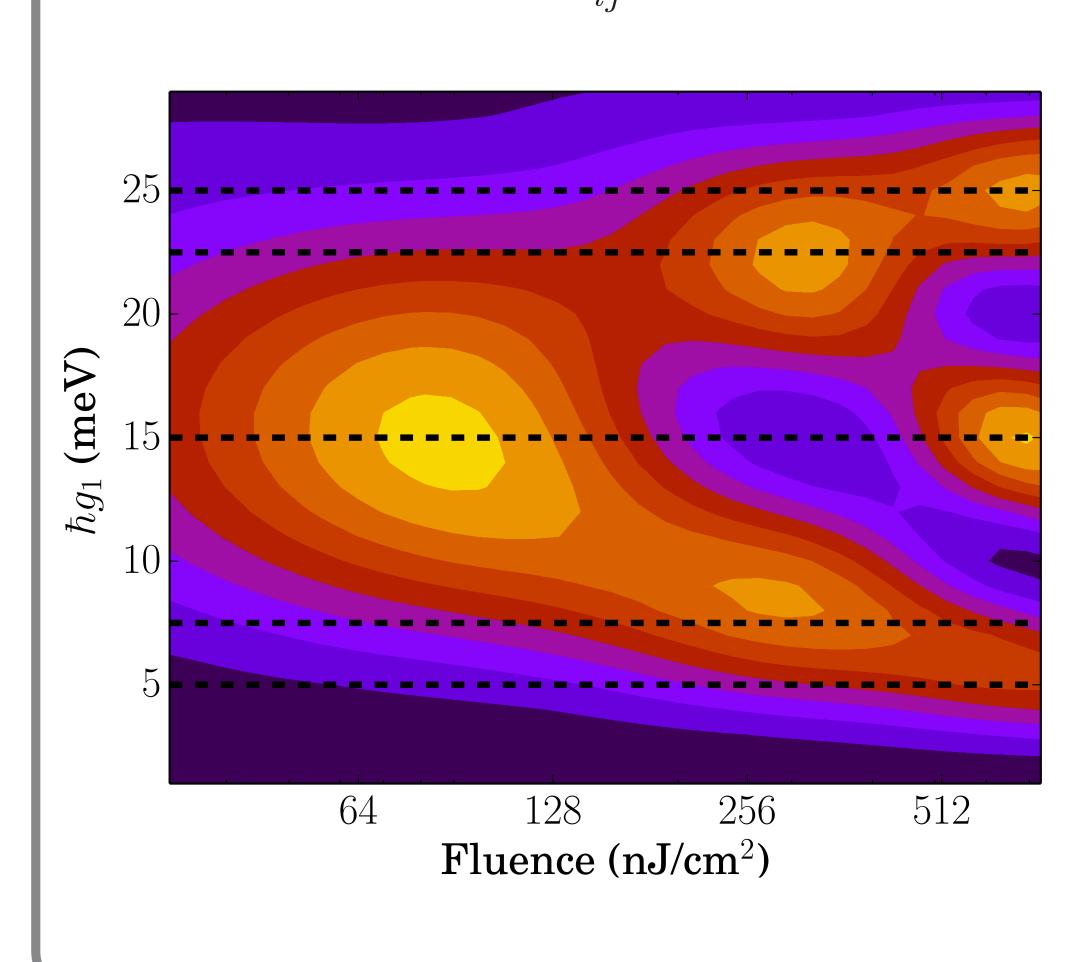
Pairwise concurrence is measured by

$$C_{ij} = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\},\,$$

where  $\lambda_k$  are the eigenvalues of a density matrix relating particles i and j

Want to identify system parameters x solving

$$\underset{x}{\text{maximize}} \sum_{i,j} C_{ij}(x)^2$$



## QAOA

Quantum approximate optimization algorithm

- Begins with an initial state  $|+\rangle^{\otimes n}$
- Quantum evolution is performed by applying two alternating operators based on the cost Hamiltonian  $H_C$  and mixing Hamiltonian  $H_M$

$$|\psi(\theta)\rangle = |\psi(\beta, \gamma)\rangle$$

$$= e^{-i\beta_p H_M} e^{-i\gamma_p H_C} \cdots e^{-i\beta_1 H_M} e^{-i\gamma_1 H_C} |+\rangle^{\otimes n}$$

• The objective function is the energy of  $H_C$  in the state  $|\psi(\beta,\gamma)\rangle$ :

$$f(\beta, \gamma) = -\langle \psi(\beta, \gamma) | H_C | \psi(\beta, \gamma) \rangle$$

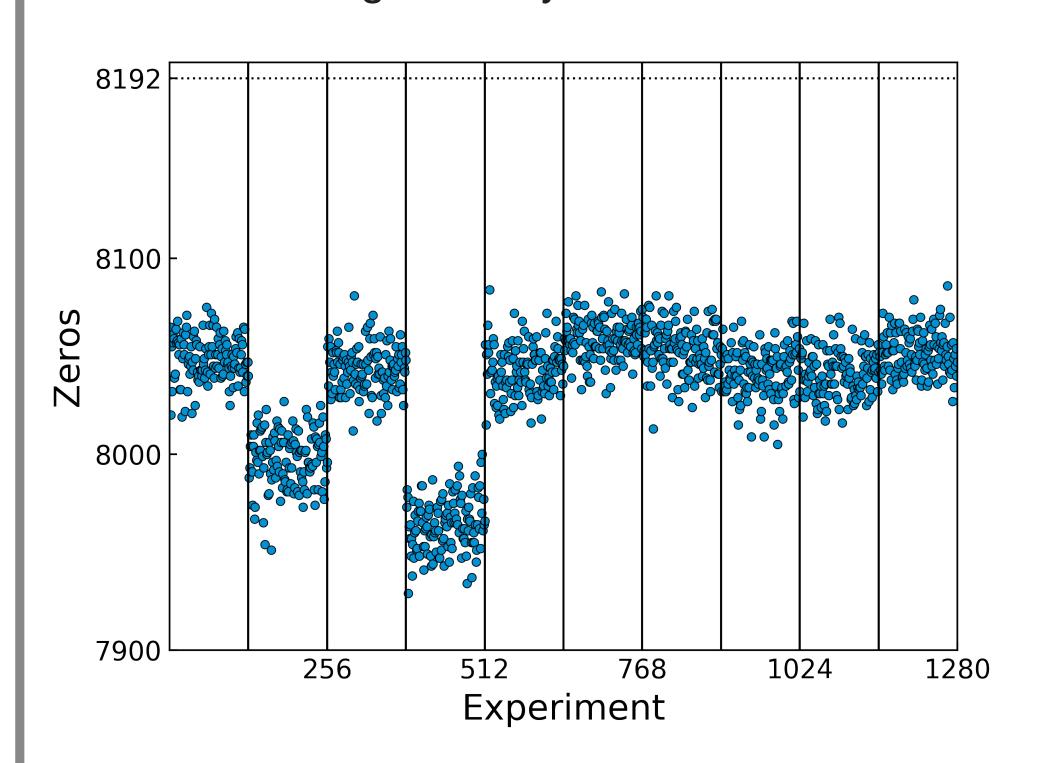
- For a small number of steps, p, the quantum evolution can be performed on NISQ devices
- QAOA's performance depends critically on the quality of angles of rotation produced by the classical optimizer
- The QAOA objective contains many suboptimal local optima. This motivates the use of a multistart framework

## Time-varying control

- 10 jobs on an IBM 20-qubit chip on 3/23/19
- Each job consists of 128 identical experiments:

## repeat 8192 times

- Prepare zero state on qubit 0
  Read out
- Counts drift significantly over time:



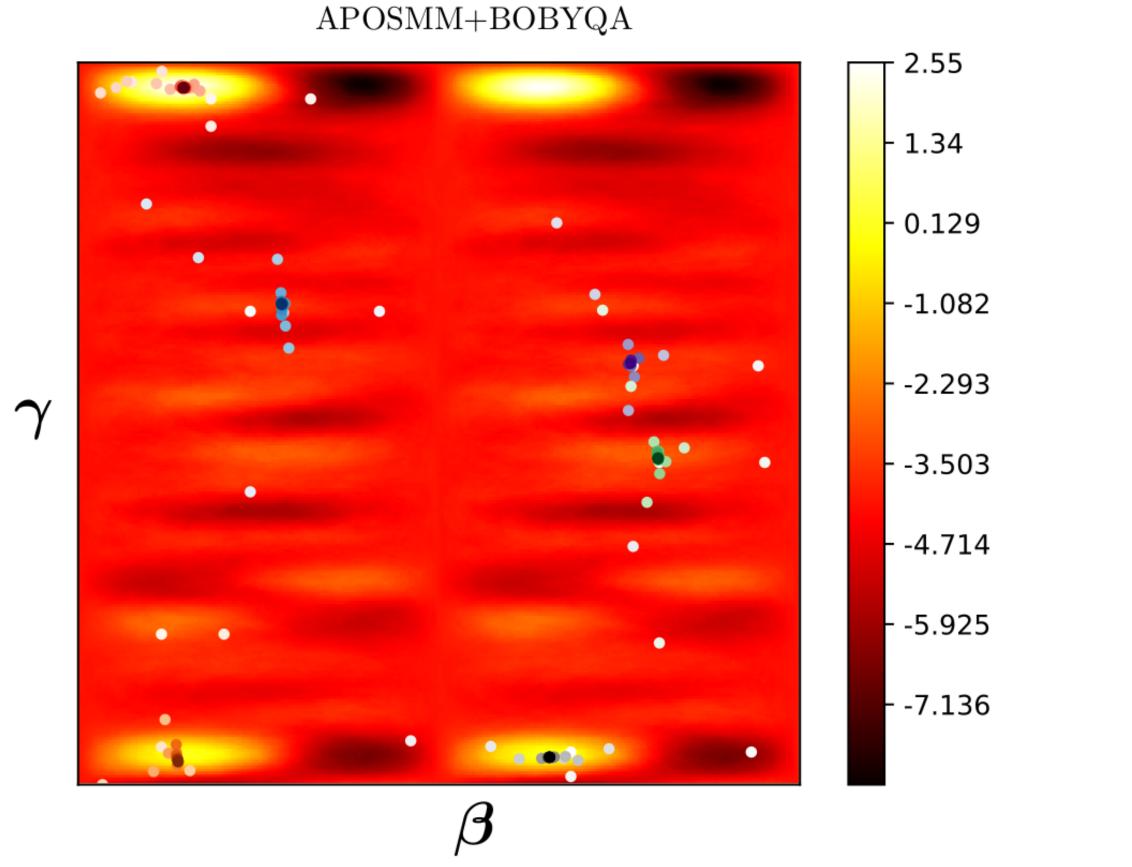
Currently developing a Bayesian method for optimizing functions with noise that depends on time and input parameters

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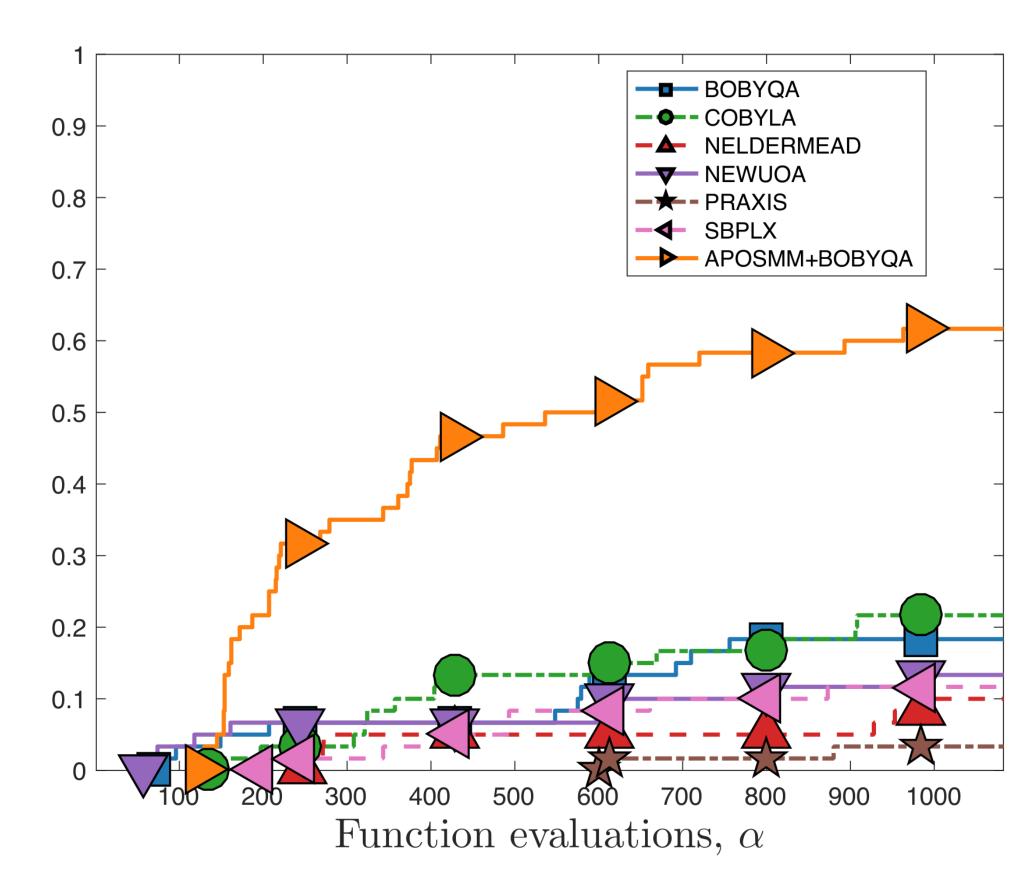
May want to cut a circuit because:

- The number of physical qubits on NISQ devices limit the size of executable quantum circuits
- Hardware noise and qubit decoherence degrade longer output from longer circuits
- Need to identify nontrivial connectivity in a quantum circuit
- Want to apply intermediate error detection
- Wish to classically simulate a portion of a circuit

# Comparing classical optimizers on QAOA

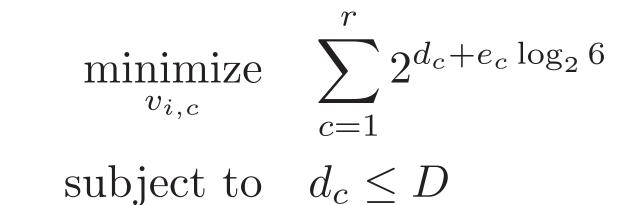


QAOA objective surface and points sampled by APOSMM+BOBYQA for a graph clustering problem



Data profiles for different classical optimizers on benchmark graph clustering problems with  $p=2\,$ 

## Clustering problem



and other constraints

### where

- $d_c$  is the number of qubits required for cluster c
- $e_c$  is the number of incoming edges to cluster c
- $x_{i,c} = 1$  if vertex i is assigned to cluster c

Larson & Wild. Asynchronously parallel optimization solver for finding multiple minima. Math. Prog. Comp. 10(3). 2018

Shaydulin, Safro, & Larson. Multistart methods for quantum approximate optimization. IEEE HPEC. 2019

Hudson, Larson, Wild, & Bindel. libEnsemble. 2019

Otten, Larson, Min, Wild, Pelton, & Gray. Origins and optimization of entanglement in plasmonically coupled quantum dots. Phys. Rev. A. 2016